Comment on "Monte Carlo Evaluation of Functional Integrals Using Coherent-State Slater Determinants"

In a recent Letter,[1] Avishai and Richert proposed a Monte Carlo evaluation of many-fermion functional integrals using real coherent-state Slater determinants. They conjectured that, in the stochastic evaluation of the mean value of the Hamiltonian H,

$$\langle H\rangle = \frac{\int D(x) H(x) \exp[-S(x)]}{\int D(x) \exp[-S(x)]}, \quad (1)$$

it is sufficient to consider only those real coherent-state Slater determinants $|x\rangle$ for which the action is real; that is, the integrand of the denominator is positive. Here, the action S consists of a dynamic term involving the matrix elements of the Hamiltonian between states at successive times and a kinematic term involving the logarithms of the overlaps of these states and the integration measure. As these overlaps can be negative, the integrand of the denominator can generally have both signs. If the positivity conjecture were correct, the evaluation of (1) would then be reduced to the sampling of a positive-definite probability density. Avishai and Richert tested this method in a simple four-level two-fermion model and claimed that it successfully reproduced the exact ground-state energy.

We would like to present briefly the results of our own investigations of this problem. First, we have obtained the computer code used in the calculations of Ref. 1 and have verified that we can reproduce the results presented there.[2] However, further calculations with this code (such as changing the step in x used in the Metropolis algorithm) indicated that the original step size used in Ref. 1 was far too small, resulting in a sampling of Slater determinants only in a small neighborhood about the state from which the random walk was initiated. The original step size results in only 5×10^{-2} of the moves being rejected because of a change in the action and essentially *none* are rejected because an overlap becomes negative; one expects that some 50% of an unbiased random sampling of phase space will lead to such a change in sign. The published fact that there are several local minima in the action from which the random walk cannot escape (and which lead to different values for the energy) also casts doubt on the validity of the Metropolis algorithm used to sample the probability density, and hence on the conclusions drawn in Ref. 1.

In order to test the positivity conjecture while at the same time avoiding any bias due to the inaccurate Metropolis sampling of a probability density with multiple (and perhaps disjoint) maxima, we have performed Monte Carlo calculations for the model of Ref. 1 in an alternative path-integral representation[3] which uses a resolution of unity for a system of A fermions in a B-dimensional single-particle basis of the form

$$1 = C\int D[\varphi] \prod_{i\le j} \delta(\langle\varphi_i|\varphi_j\rangle - \delta_{ij})|\Phi\rangle\langle\Phi|. \quad (2)$$

Here, C is a normalizing constant and the integral is over the A real single-particle wave functions φ making up the many-body Slater determinant Φ. This form is particularly convenient as an unbiased Metropolis move can be made simply by choosing the A φ's randomly on a B-dimensional hypersphere and then orthonormalizing them via a Gram-Schmidt process; acceptance or rejection then depends on the change in the action in the usual way. We find that some 50% of such moves lead to a change in sign of the overlap between determinants at two successive times, indicating that configurations of the system are being properly sampled. For calculations with $\beta = 0.5$ and $N = 50$ or 100 time slices, we find that $\approx 60\%$ of the remaining moves are accepted when changes in S are considered. If only the positive contributions to the integrals are retained, the average energy [Eq. (1)] is found to be 8.41 ± 0.23 and 14.90 ± 0.37 for $N = 50$ and 100, respectively. These values are to be compared with the exact answer, 4.50, which would be obtained (with a very large statistical error!) if both positive and negative contributions were retained. The dependence we find on the number of time slices is not too surprising since the retention of only positive integrands completely destroys the resolution of unity at each time slice.

In view of the results presented above, it does not appear that the conjecture of Ref. 1 leads to a tractable Monte Carlo method for treating many-fermion systems.

T. Troudet
S. E. Koonin
W. K. Kellogg Radiation Laboratory
California Institute of Technology
Pasadena, California 91125

Received 3 June 1983
PACS numbers: 02.70.+d, 21.60.-n, 31.15.+q

[1] Y. Avishai and J. Richert, Phys. Rev. Lett. 50, 1175 (1983).

[2] We thank Y. Avishai for sending us a listing and sample output of his computer code.

[3] T. Troudet and S. E. Koonin, to be published.

